NAMBE

Room Cummings Ballroom - Session NAMBE1-WeM

Nitrides

Moderator: Kevin Vallejo, Idaho National Laboratory

8:15am **NAMBE1-WeM-1 Welcome & Sponsor Thank Yous**,

8:30am **NAMBE1-WeM-2 Tunnel Junction Engineered MBE-grown Nanowires: Toward Self-Powered, Dual-Wavelength Photoelectrochemical Photodetectors for Secure and Efficient Underwater Wireless Sensors Networks**, *S. Zhao,* ***Milad Fathabadi,*** McGill University, Canada

The development of underwater wireless sensor networks (UWSNs) is increasingly critical for monitoring the ocean environment, where the demand for robust, secure, and energy-efficient technologies is at its highest peak. Self-powered, wavelength-distinguishable photodetectors (PDs) are appealing to meet the demands of UWSNs, offering low energy consumption and maintenance costs and enabling complex data encryption via light. The self-powered and wavelength-distinguishable photodetection can be more easily achieved with photoelectrochemical (PEC) PDs, thanks to their operating principle that leverages semiconductor-electrolyte interactions that offer greater flexibility in tuning the photoresponse. Semiconductor p-n heterojunctions with suitable bandgaps could enable wavelength-distinguishable photodetection based on photocurrent polarity (negative for p-type and positive for n-type). However, the built-in electric field at the p-n junction prevents reaching the desired dual photocurrent polarity (Figure S1a).

Herein, we designed a III-nitride nanowire p-n heterojunction embedded with a tunnel junction (TJ) to overcome this challenge, and achieved the first self-powered, wavelength-distinguishable PEC-PDs. The TJ not only reverses the direction of the unfavorable electric field but also facilitates the transport of photogenerated carriers (Figure S1b). Figure S1c shows the STEM images of high-quality n-GaN/p-InGaN nanowires with a n^{++}-GaN/InGaN/p^{++}-GaN TJ embedded for UV-visible wavelength detection, and the response is shown in Figure S1d. It is seen that, self-powered, wavelength-distinguishable photodetection is obtained at 405 and 302 nm. Moreover, our devices exhibit high responsivities in the mA/W range for both wavelengths, with ultrafast response times of less than 10 ms for 405 nm and 20-30 ms for 302 nm light. The ability of this PEC-PD to function without external electrical power and to distinguish between UV and blue light wavelengths paves the way for more secure data transmission in UWSNs with blue light, the most transparent wavelength in the ocean.

8:45am **NAMBE1-WeM-3 MBE Growth of n-type AlN and Defect Characterization Using Deep UV Photoluminescence**, ***Neeraj Nepal,*** *M. Hardy, A. Lang, B. Downey, D. Katzer, E. Jin, V. Gokhale, T. Growden, D. Meyer, V. Wheeler,* Naval Research Laboratory

AlN has a bandgap of ~6.2 eV resulting in a large critical electric field breakdown (>15 MV/cm), leading to a higher Baliga's and Johnson's figure-of-merit for power and RF devices, respectively. Further, AlN possesses a high saturation velocity (~$2x10^7$ cm/s) and high thermal conductivity (~319 $Wm^{-1}K^{-1}$). Realizing the full potential of this material in electronic devices requires the ability to tailor the electrical conductivity in active AlN layers through impurity doping.

Due to the large bandgap and lower formation energy of native point defects, which serves as carrier compensating centers, impurity doping in AlN has been challenging, and thus there is limited understanding of how to control and implement repeatable impurity doping in AlN-based devices. Deep ultraviolet photoluminescence (DUVPL) is a crucial tool to understand and optimizing the AlN growth process for electrical applications, allowing for the correlation of impurity defects, near-bandedge emission bands and conductivity.

In this presentation, we report on the growth of ~300 to 500 nm thick Si-doped AlN films by plasma-assisted molecular beam epitaxy (MBE). The AlN thin films were grown on AlN/sapphire and bulk AlN templates from different vendors using a metal modulated epitaxy approach and studied the resulting films using room temperature DUVPL, x-ray diffraction (XRD), atomic force microscopy (AFM) and van der Pauw resistivity measurements. Cross-sectional transmission electron microscopy (TEM) measurements were carried out on selected samples along (1 0 $\bar{1}$ 0) and (1 1 $\bar{2}$ 0) orientations to assess the epitaxial material quality and defect density.

All AlN substrates underwent an ex-situ chemical clean and in-situ Al-absorption and desorption technique before nucleating AlN films. The evolution of the substrate surface during the in-situ clean was monitored with reflection high-energy electron diffraction and verified to be oxygen free using TEM and electron energy loss spectroscopy. DUVPL measurements of MBE AlN layers, using above bandgap excitation (at 6.458 eV), show that unintentionally-doped AlN films have strong band-edge emission and no impurity bands. After Si doping, an impurity band near 3.67 eV due to an Al-vacancy Si-complex appears and band-edge emission at 6.03 eV (for AlN/sapphire) decreases. Van der Pauw resistivity measurements show that the AlN:Si films grown at optimized growth conditions on all substrates are conductive. For AlN layers grown under similar conditions, conductive AlN films have lower intensity impurity bands. Results correlating DUVPL, XRD, AFM, TEM and resistivity measurements for the full parameter space will be discussed.

9:00am **NAMBE1-WeM-4 Evolution of AlN: from 1 nm Nitridation to 2 µm by Molecular Beam Epitaxy**, *M. Liao, D. Luccioni, K. Huynh, Y. Wang, L. Matto,* University of California Los Angeles*; H. Ahmad,* Georgia Institute of Technology*; Z. Zhang,* Argonne National Laboratory*; W. Doolittle,* Georgia Institute of Technology*;* ***Mark Goorsky,*** University of California Los Angeles

The structural evolution of AlN from ~1 nm nitridation on (0001) sapphire followed by up to 2 µm of molecular beam epitaxial growth at 800 °C was studied. An ~80 nm Al cap was deposited for each sample after nitridation or epitaxial growth of various AlN thicknesses. In-situ, post-growth annealing at 800 °C improved the structural characteristics of the AlN. The structures are important for understanding the role of interfacial defects on thermal transport across AlN interfaces.

The initial nitridation of the sapphire substrate surface produced a 1.6 nm AlN layer. Synchrotron X-ray measurements revealed only {0001} surface planes and a narrow (0002) rocking curve width of ~30". The (0001) orientation was maintained during subsequent AlN growth. This contrasts with AlN growths on non-nitrided sapphire where (0001) and (10$\underline{1}$2) islands formed [1] initially. We show nitridation of (0001) sapphire enables only (0001) AlN formation and hinders the nucleation of other orientations, resultingin less defective AlN|Al_2O_3 interfaces. Symmetric X-ray rocking curves for all thicknesses of AlN exhibit two-peak components. Two-peak-component rocking curves have been reported by other studies [2], but the components' characteristics had not previously been determined. By observing the behavior of each rocking curve component at different orders of {000ℓ} symmetric reflections, it is ascertained that one component is attributed to lattice tilt (~30" for 1.6 nm to 230 nm AlN films) or mosaic and the other is due to lateral coherence length (which increases with increasing AlN thickness). In situ annealing at the growth temperature resulted in further rocking curve width reduction for the broad component, which corresponds to longer coherence lengths and therefore higher quality material as well. More insightfully, the improvement in film quality is due to the time spent at elevated temperatures rather than the act of growing thicker films. For example, the broad component width of the as-grown 68 nm film was 640" and decreased to 480" after annealing at the growth temperature to match the growth time to achieve a 120 nm thick film. The annealed 68 nm film width matched the as-grown 120 nm film peak width. Studying the evolution of films from ~1 nm to µm regime is essential towards refining epitaxial growth strategies and understanding the role of structural characteristics on the thermal transport across interfaces.

The authors acknowledge support from the Office of Naval Research, grant No. N00014-18-1-2429.

[1] J.R.Heffelfinger, et al., J.Appl.Phys., 85(1) 466 (1999).

[2] J.Wang, et al., Scientific Reports, 7 42747 (2017).

9:15am **NAMBE1-WeM-5 Addressing the High Coercive Field of $Sc_xAl_{1-x}N$ via Magnesium Doping in Molecular Beam Epitaxy**, ***Samuel Yang,*** *D. Wang, D. Wang, Z. Mi,* University of Michigan, Ann Arbor

Wurtzite nitride ferroelectrics have been the centre of much attention since their experimental introduction in 2019. The incorporation of rare earth elements, such as Sc and Y, into the conventional III-nitride materials AlN and GaN can transform them into ferroelectric materials by flattening the energy landscape for polarity switching between the metal-polar and nitrogen-polar states. Compared to conventional oxide ferroelectrics, these materials have been shown to offer higher Curie temperatures, larger remanent polarisations, and greater scalability. Advances in molecular

beam epitaxy (MBE) have led to demonstrations of high-quality monocrystalline $Sc_xAl_{1-x}N$ and $Sc_xGa_{1-x}N$. Together with amplified piezoelectricity and optical activeness, these materials harbour great promise for next-generation reconfigurable electronics and optoelectronics, memory, and piezoelectric and acoustic devices. Despite these prospects, ferroelectric nitrides face numerous challenges, especially considering stringent demands within the modern semiconductor industry. Among these challenges is the high coercive field (E_c) of $Sc_xAl_{1-x}N$. Although some technologies benefit from higher E_c, the increased switching voltage can promote defect formation and accumulation, as well as exacerbate leakage currents and diminish endurance cycles. As a first step towards realising $Sc_xAl_{1-x}N$ with lower E_c, an investigation into the epitaxial growth and ferroelectric properties of Mg-doped $Sc_xAl_{1-x}N$ is performed. Samples of $Sc_{0.2}Al_{0.8}N$ doped with various concentrations of Mg are grown via plasma-assisted MBE on a GaN-on-sapphire template. Reflection high-energy electron diffraction (RHEED) and atomic force microscopy (AFM) confirm excellent crystallinity and morphology, with surface *rms* roughness of ~0.5 nm over 25 μm^2 scan areas across multiple samples. Quasi-static J-E (current density vs electric field) measurements reveal clear reduction in E_c with Mg incorporation. Further P-E (polarisation vs electric field) measurements corroborate unambiguous ferroelectric switching and demonstrate moderate remanent polarisations of ~70-80 $\mu C\ cm^{-2}$. The initial demonstration of Mg-doped $Sc_xAl_{1-x}N$ to ameliorate faced challenges opens exciting new avenues through which nitride ferroelectrics can be tuned and enhanced for multifarious applications via doping engineering. Further study is anticipated to optimise the effects of and unveil the mechanisms behind E_c reduction with Mg doping.

9:45am **NAMBE1-WeM-7 Epitaxial Integration of Transition-Metal Nitrides with Cubic Gallium Nitrid*e, Zach Cresswell,*** *N. Fessler, T. Garrett, K. Vallejo, B. May,* Idaho National Laboratory

GaN is ubiquitous in the optoelectronics industry in its thermodynamically stable wurtzite structure, but it also has a metastable zinc blende allotrope that is less explored and more difficult to synthesize. One of the potential advantages of cubic-GaN (c-GaN) is the simplified interfacial symmetry with the other cubic transition metal nitrides, which are of interest for an assortment of applications requiring high chemical and thermal stability, high hardness, superconductivity, or plasmonic properties. The shared cubic symmetry would allow for easier integration of the nitrides with a wide-bandgap semiconductor.

This work will discuss the synthesis of epitaxial c-GaN on 3C-SiC substrates and its integration with known superconducting nitrides via molecular beam epitaxy. The hexagonal-free nature of the c-GaN, and the epitaxial relationship of it and the transition metal nitrides, are confirmed via *in-situ* reflection high energy electron diffraction, *ex-situ* X-ray diffraction, photoluminescence, and transition electron microscopy. The electrical transport of the transition metal nitrides grown on c-GaN(001) is compared to growth directly on 3C-SiC(001) and c-plane hexagonal GaN. Epitaxial synthesis of cubic wide-bandgap and superconducting metallic nitrides under similar growth conditions opens a new world of possibilities in band engineering, as well as the ability to create new device structures for areas such as metamaterials, quantum computing, and condensed matter physics.

10:00am **NAMBE1-WeM-8 Epitaxial Growth of High ScN Fraction ScAlN on (111) Si*, Matthew Hardy,*** *E. Jin, N. Nepal, B. Downey, V. Gokhale, D. Katzer, V. Wheeler, V. Wheeler,* U.S. Naval Research Laboratory

ScAlN thin films have attracted significant attention due to their 5× increase in piezoresponse over AlN for $Sc_xAl_{1-x}N$ compositions of x = 0.43 [1], leading to applications in 5G filters and RF electronics. Epitaxial growth of ScAlN on Si enables the use of mature MEMS processing technology.

In this work, we demonstrate the growth of $Sc_xAl_{1-x}N$ layers on AlN nucleation layers (NL) on 100-mm (111) Si wafers with x up to 0.40 using MBE. AlN NLs with III/V ratios of 0.5 and 0.8 show polycrystalline ring segments in reflection high-energy electron diffraction (RHEED), III/V of 0.93 gives a streaky RHEED pattern with slight spot-modulation and no apparent etching of the Si substrate, seen in AlN with III/V > 1. Subsequent growth of $Sc_{0.40}Al_{0.60}N$ layers exhibit similar features to the underlying AlN NL, with a single phase wurtzite RHEED pattern only for the AlN III/V = 0.93 sample.

Several ScAlN samples were grown at 410 °C, varying both the Sc and Al flux to allow changes in the III/V ratio for a fixed composition. At low III/V ≤ 0.8, rings appear in the RHEED pattern suggesting the presence of polycrystalline domains. At III/V around 0.95, the ScAlN RHEED is free of extraneous features. At III/V ≥ 1.0 the RHEED pattern broadens and forms indistinct dual-ring-segments. This is the first demonstration of both a lower and upper bound to the high ScN fraction growth space, as well as identification of characteristic RHEED patterns, and is distinct from the III/V ratio behavior at low ScN fraction ($x \leq 0.2$).

A graded ScAlN nucleation layer, previously demonstrated for ScAlN/SiC, is further investigated for ScAlN on Si. A 25-nm grade from x = 0.3→0.38 reduces the 0002 X-ray diffraction (XRD) rocking curve full-width at half maximum (FWHM) from 0.90° to 0.73°, and reduces the film stress from 0.92 to 0.59 GPa. Increasing the grade thickness for a fixed total thickness of 133 nm leads to a small reduction in FWHM (0.71°) and stress (0.46 GPa) for a 75 nm grade, with little change for a 115 nm grade.

An optimized ScAlN/AlN/Si sample, having a 10-nm AlN NL, a 20-nm graded 0.32 to 0.40 ScAlN nucleation layer, and a 100-nm $Sc_{0.40}Al_{0.60}N$ layer, shows a clean wurtzite RHEED pattern throughout growth, a FWHM of 1.1°, and an rms roughness of 0.57 nm. Atomic force microscopy height and phase images show no indication of anomalously oriented grains. Such thin, high structural and phase purity films are well suited to high frequency RF MEMS applications.

[1]M. Akiyama, K. Kano, and A. Teshigahara, *Appl. Phys. Lett.,* **95**, 162107 (2009).

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